

WEST Search History

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DATE: Friday, March 11, 2005

<u>Hide?</u>	<u>Set Name</u>	<u>Query</u>	<u>Hit Count</u>
<i>DB=PGPB,USPT; PLUR=YES; OP=ADJ</i>			
<input type="checkbox"/>	L6	l4 and (alkoxy or methoxide or ethoxide or propoxide or butoxide)	3
<input type="checkbox"/>	L5	epoxytrifluoropropionic acid	0
<input type="checkbox"/>	L4	l1 and l3	6
<input type="checkbox"/>	L3	epoxy or epoxid\$	261630
<input type="checkbox"/>	L2	epoxy oe epoxid\$	0
<input type="checkbox"/>	L1	trifluoromethacrylic acid	21

END OF SEARCH HISTORY

[REDACTED]
d his

(FILE 'HOME' ENTERED AT 15:08:59 ON 11 MAR 2005)

FILE 'REGISTRY' ENTERED AT 15:09:16 ON 11 MAR 2005

L1 STRUCTURE uploaded
L2 STRUCTURE uploaded
L3 STRUCTURE uploaded
L4 1 S L1
L5 22 S L1 FULL
L6 0 S L2
L7 3 S L2 FULL
L8 0 S L3
L9 2 S L3 FULL

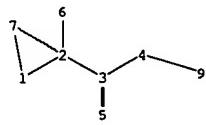
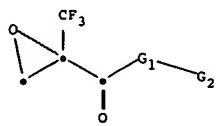
FILE 'CAPLUS' ENTERED AT 15:12:53 ON 11 MAR 2005

L10 10 S L5
L11 3 S L7
L12 1 S L9
L13 16 S ?TRIFLUOROMETHACRYLIC ACID?
L14 294484 S EPOXY? OR EPOXID?
L15 1 S L13 AND L14
L16 20 S ?OXIRANE CARBOXYLIC ACID?
L17 0 S L13 AND L16
L18 0 S ?EPOXYTRIFLUOROPROPIONIC ACID
L19 0 S L13 AND (?ALKOXIDE OR ?METHOXIDE OR ?PROPOXIDE O

FILE 'REGISTRY' ENTERED AT 15:20:23 ON 11 MAR 2005

FILE 'CASREACT' ENTERED AT 15:20:36 ON 11 MAR 2005

L20 STRUCTURE uploaded
L21 STRUCTURE uploaded
L22 0 S L20
L23 0 S L20 FULL
L24 0 S L21
L25 0 S L21 FULL



chain nodes :
3 4 5 6 9

ring nodes :
1 2 7

chain bonds :
2-3 2-6 3-4 3-5 4-9

ring bonds :
1-2 1-7 2-7

exact/norm bonds :
3-4 3-5 4-9

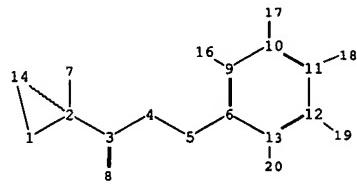
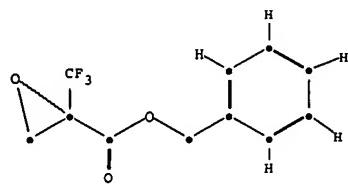
exact bonds :
1-2 1-7 2-3 2-6 2-7

isolated ring systems :
containing 1 :

$G_1:\text{O}, \text{S}, \text{NH}$

$G_2:\text{Cb}, \text{Ak}, \text{Ph}$

Match level :
1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 9:CLASS

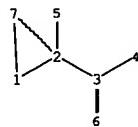
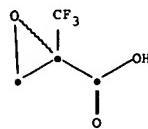


```

chain nodes :
 3 4 5 7 8 16 17 18 19 20
ring nodes :
 1 2 6 9 10 11 12 13 14
chain bonds :
 2-3 2-7 3-4 3-8 4-5 5-6 9-16 10-17 11-18 12-19 13-20
ring bonds :
 1-2 1-14 2-14 6-9 6-13 9-10 10-11 11-12 12-13
exact/norm bonds :
 1-2 1-14 2-14 3-4 3-8 4-5
exact bonds :
 2-3 2-7 5-6 9-16 10-17 11-18 12-19 13-20
normalized bonds :
 6-9 6-13 9-10 10-11 11-12 12-13
isolated ring systems :
  containing 6 :

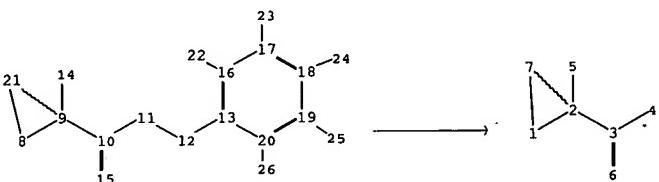
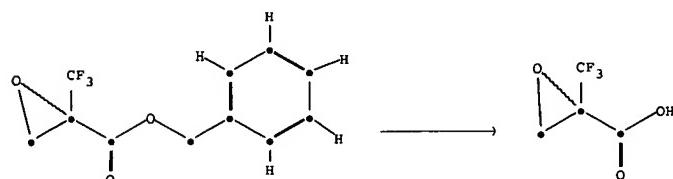
Match level :
 1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:CLASS 8:CLASS 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS

```



```
chain nodes :
 3 4 5 6
ring nodes :
 1 2 7
chain bonds :
 2-3 2-5 3-4 3-6
ring bonds :
 1-2 1-7 2-7
exact bonds :
 1-2 1-7 2-3 2-5 2-7
normalized bonds :
 3-4 3-6
isolated ring systems :
  containing 1 :

Match level :
 1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom
```

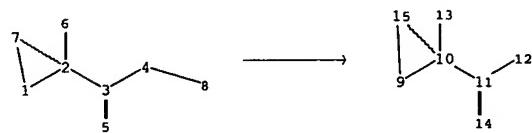
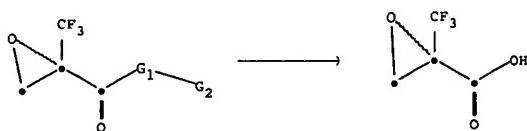


```

chain nodes :
 3 4 5 6 10 11 12 14 15 22 23 24 25 26
ring nodes :
 1 2 7 8 9 13 16 17 18 19 20 21
chain bonds :
 2-3 2-5 3-4 3-6 9-10 9-14 10-11 10-15 11-12 12-13 16-22 17-23
 18-24 19-25 20-26
ring bonds :
 1-2 1-7 2-7 8-9 8-21 9-21 13-16 13-20 16-17 17-18 18-19 19-20
exact/norm bonds :
 10-11 10-15 11-12
exact bonds :
 1-2 1-7 2-3 2-5 2-7 8-9 8-21 9-10 9-14 9-21 12-13 16-22 17-23
 18-24 19-25 20-26
normalized bonds :
 3-4 3-6 13-16 13-20 16-17 17-18 18-19 19-20
isolated ring systems :
 containing 1 : 8 : 13 :

Match level :
 1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 13:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS
26:CLASS
fragments assigned product role:
 containing 1
fragments assigned reactant/reagent role:
 containing 8

```



```

chain nodes :
 3 4 5 6 8 11 12 13 14
ring nodes :
 1 2 7 9 10 15
chain bonds :
 2-3 2-6 3-4 3-5 4-8 10-11 10-13 11-12 11-14
ring bonds :
 1-2 1-7 2-7 9-10 9-15 10-15
exact/norm bonds :
 1-2 1-7 2-7 3-4 3-5 4-8 9-10 9-15 10-15
exact bonds :
 2-3 2-6 10-11 10-13
normalized bonds :
 11-12 11-14

G1:O,S,NH

G2:Cb,Ak,Ph

Match level :
 1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:CLASS 9:Atom
 10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom
fragments assigned product role:
  containing 9
fragments assigned reactant/reagent role:
  containing 1

```

L1 STRUCTURE UPLOADED

=>
Uploading C:\Program Files\Stnexp\Queries\686-2.str

L2 STRUCTURE UPLOADED

=>
Uploading C:\Program Files\Stnexp\Queries\686-3.str

L3 STRUCTURE UPLOADED

=> s 11
SAMPLE SEARCH INITIATED 15:10:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 12 TO ITERATE

100.0% PROCESSED 12 ITERATIONS
SEARCH TIME: 00.00.01

1 ANSWERS

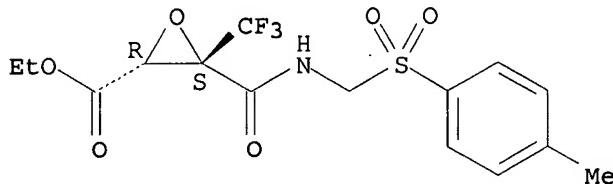
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 33 TO 447
PROJECTED ANSWERS: 1 TO 80

L4 1 SEA SSS SAM L1

=> d scan

L4 1 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 3-[[[(4-methylphenyl)sulfonyl]methyl]amino]carbon
yl]-3-(trifluoromethyl)-, ethyl ester, trans- (9CI)
MF C15 H16 F3 N O6 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s 11 full
FULL SEARCH INITIATED 15:10:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 263 TO ITERATE

100.0% PROCESSED 263 ITERATIONS
SEARCH TIME: 00.00.01

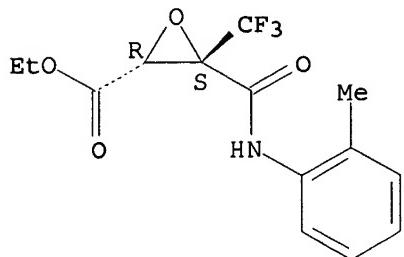
22 ANSWERS

L5 22 SEA SSS FUL L1

=> d scan

L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 3-[[[(2-methylphenyl)amino]carbonyl]-3-
(trifluoromethyl)-, ethyl ester, trans- (9CI)
MF C14 H14 F3 N O4

Relative stereochemistry.

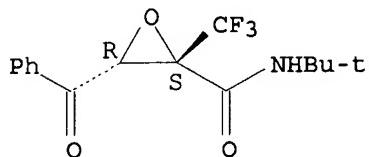


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxamide, 3-benzoyl-N-(1,1-dimethylethyl)-2-(trifluoromethyl)-,
trans- (9CI)
MF C15 H16 F3 N O3

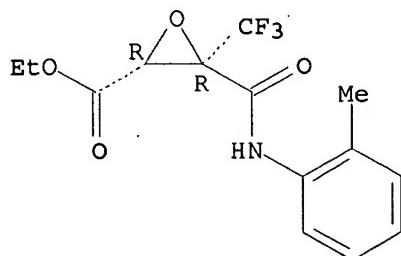
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 3-[[[(2-methylphenyl)amino]carbonyl]-3-
(trifluoromethyl)-, ethyl ester, cis- (9CI)
MF C14 H14 F3 N O4

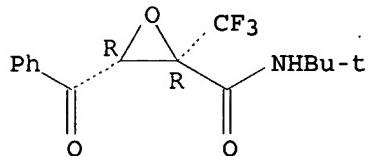
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxamide, 3-benzoyl-N-(1,1-dimethylethyl)-2-(trifluoromethyl)-,
cis- (9CI)
MF C15 H16 F3 N O3

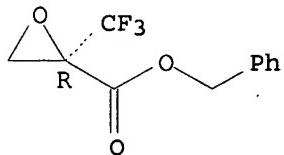
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

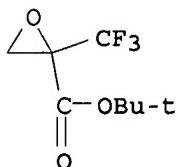
L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 2-(trifluoromethyl)-, phenylmethyl ester, (2R)-
(9CI)
MF C11 H9 F3 O3

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

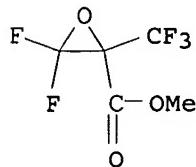
L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 2-(trifluoromethyl)-, 1,1-dimethylethyl ester
(9CI)
MF C8 H11 F3 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

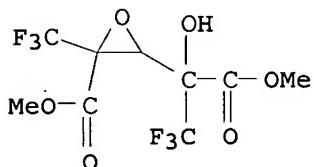
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 3,3-difluoro-2-(trifluoromethyl)-, methyl ester
(9CI)
MF C5 H3 F5 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

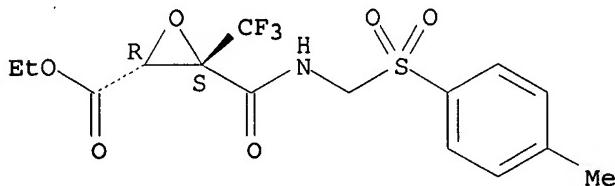
L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiraneacetic acid, α -hydroxy-3-(methoxycarbonyl)- α ,3-bis(trifluoromethyl)-, methyl ester (9CI)
MF C9 H8 F6 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 3-[[[[(4-methylphenyl)sulfonyl]methyl]amino]carbon yl]-3-(trifluoromethyl)-, ethyl ester, trans- (9CI)
MF C15 H16 F3 N O6 S

Relative stereochemistry.



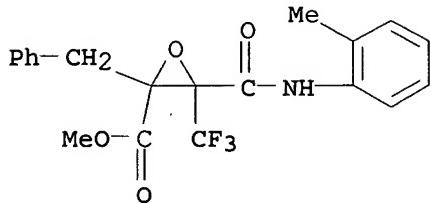
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 3-[(2-methylphenyl)amino]carbonyl]-2-

[REDACTED]

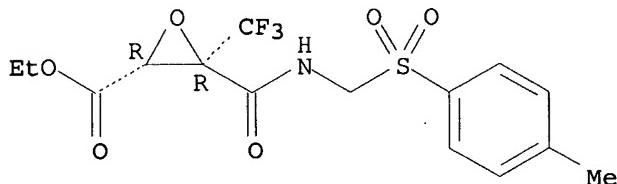
(phenylmethyl)-3-(trifluoromethyl)-, methyl ester (9CI)
MF C₂₀ H₁₈ F₃ N O₄



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 3-[[[[(4-methylphenyl)sulfonyl]methyl]amino]carbon
yl]-3-(trifluoromethyl)-, ethyl ester, cis- (9CI)
MF C₁₅ H₁₆ F₃ N O₆ S

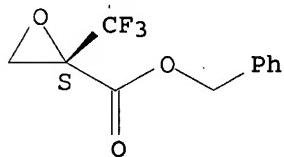
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 2-(trifluoromethyl)-, phenylmethyl ester, (2S)-
(9CI)
MF C₁₁ H₉ F₃ O₃

Absolute stereochemistry. Rotation (+).



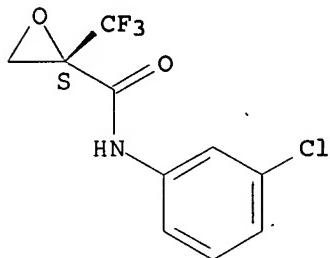
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxamide, N-(3-chlorophenyl)-2-(trifluoromethyl)-, (2S)- (9CI)

MF C10 H7 Cl F3 N O2

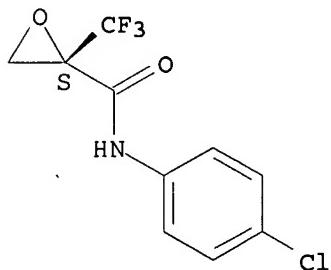
Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

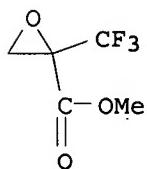
L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxamide, N-(4-chlorophenyl)-2-(trifluoromethyl)-, (2S)- (9CI)
MF C10 H7 Cl F3 N O2

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 22 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 2-(trifluoromethyl)-, methyl ester (9CI)
MF C5 H5 F3 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s 12

SAMPLE SEARCH INITIATED 15:11:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2 TO 124
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L2

=> s 12 full
FULL SEARCH INITIATED 15:11:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 49 TO ITERATE

100.0% PROCESSED 49 ITERATIONS
SEARCH TIME: 00.00.01

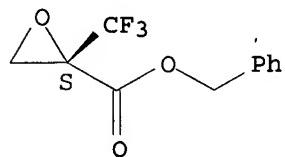
3 ANSWERS

L7 3 SEA SSS FUL L2

=> d scan

L7 3 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 2-(trifluoromethyl)-, phenylmethyl ester, (2S)-
(9CI)
MF C11 H9 F3 O3

Absolute stereochemistry. Rotation (+).

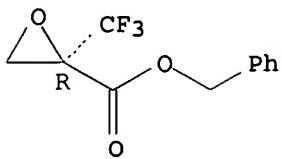


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L7 3 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 2-(trifluoromethyl)-, phenylmethyl ester, (2R)-
(9CI)
MF C11 H9 F3 O3

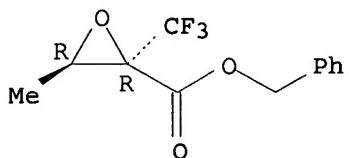
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 3 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
 IN Oxiranecarboxylic acid, 3-methyl-2-(trifluoromethyl)-, phenylmethyl ester,
 (2R,3R) - (9CI)
 MF C12 H11 F3 O3

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s 13
 SAMPLE SEARCH INITIATED 15:11:39 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00:00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 3 TO 163
 PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L3

=> s 13 full
 FULL SEARCH INITIATED 15:11:43 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 40 TO ITERATE

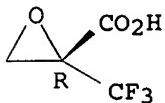
100.0% PROCESSED 40 ITERATIONS 2 ANSWERS
 SEARCH TIME: 00.00.01

L9 2 SEA SSS FUL L3

=> d scan

L9 2 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
 IN Oxiranecarboxylic acid, 2-(trifluoromethyl)-, (2R)- (9CI)
 MF C4 H3 F3 O3

Absolute stereochemistry. Rotation (-).

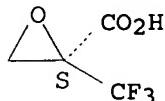


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L9 2 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Oxiranecarboxylic acid, 2-(trifluoromethyl)-, (2S)- (9CI)
MF C4 H3 F3 O3

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

E CONTENT:1840 - 6 Mar 2005 VOL 142 ISS 10

```
*****  
*  
* CASREACT now has more than 8 million reactions  
*  
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=>  
Uploading C:\Program Files\Stnexp\Queries\686-4.str
```

L20 STRUCTURE UPLOADED

```
=>  
Uploading C:\Program Files\Stnexp\Queries\686-5.str
```

L21 STRUCTURE UPLOADED

```
=> s 120  
SAMPLE SEARCH INITIATED 15:21:22 FILE 'CASREACT'  
SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS
```

```
100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS: ONLINE **COMPLETE**  
BATCH **COMPLETE**  
PROJECTED VERIFICATIONS: 0 TO 0  
PROJECTED ANSWERS: 0 TO 0
```

L22 0 SEA SSS SAM L20 (0 REACTIONS)

```
=> s 120 full  
FULL SEARCH INITIATED 15:21:28 FILE 'CASREACT'  
SCREENING COMPLETE - 3 REACTIONS TO VERIFY FROM 1 DOCUMENTS
```

```
100.0% DONE 3 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01
```

L23 0 SEA SSS FUL L20 (0 REACTIONS)

```
=> s 121  
SAMPLE SEARCH INITIATED 15:21:34 FILE 'CASREACT'  
SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS
```

```
100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS: ONLINE **COMPLETE**  
BATCH **COMPLETE**  
PROJECTED VERIFICATIONS: 0 TO 0  
PROJECTED ANSWERS: 0 TO 0
```

L24 0 SEA SSS SAM L21 (0 REACTIONS)

[REDACTED]
=> S 121 full

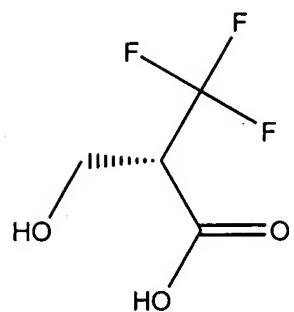
FULL SEARCH INITIATED 15:21:39 FILE 'CASREACT'
SCREENING COMPLETE - 5 REACTIONS TO VERIFY FROM

2 DOCUMENTS

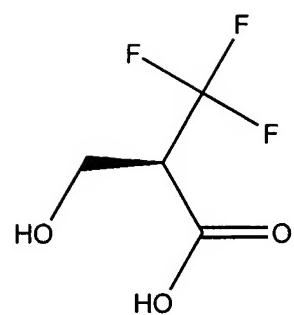
100.0% DONE 5 VERIFIED 0 HIT RXNS
SEARCH TIME: 00.00.01

0 DOCS

L25 0 SEA SSS FUL L21 (0 REACTIONS)



(S)-3,3,3-trifluoro-2-hydroxy-methylpropionic acid



(R)-3,3,3-trifluoro-2-hydroxy-methylpropionic acid